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A second orthorhombic polymorph of 2-(pyridin-4-ylmethoxy)phenol

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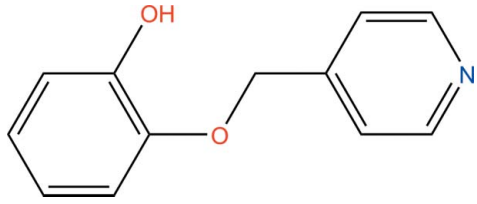
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.043; wR factor = 0.077; data-to-parameter ratio = 16.6.

The crystal structure of the title compound, $C_{12}H_{11}NO_2$, represents a new orthorhombic polymorph II of the previously reported orthorhombic form I [Zhang *et al.* (2009) *Acta Cryst.* E**65**, o3160]. In polymorph II, the six-membered rings form a dihedral angle of 13.8 (1)° [71.6 (1)° in I], and O—H···N hydrogen bonds link molecules into chains along [100], whereas the crystal structure of I features hydrogen-bonded centrosymmetric dimers.

Related literature

For details of the synthesis, see: Gao *et al.* (2004). For the crystal structure of polymorph I, see: Zhang *et al.* (2009).



Experimental

Crystal data

$C_{12}H_{11}NO_2$
M_r = 201.22
Orthorhombic, $Pca2_1$
a = 23.398 (5) Å
b = 5.8343 (12) Å
c = 7.3934 (15) Å
V = 1009.3 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 293 K
0.50 × 0.37 × 0.11 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.956, T_{max} = 0.990
8907 measured reflections
2285 independent reflections
1298 reflections with $I > 2\sigma(I)$
R_{int} = 0.066

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.077
S = 1.01
2285 reflections
138 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.15 e Å^{-3}
$\Delta\rho_{min}$ = −0.14 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N1^{i}	0.82	1.95	2.763 (2)	173

Symmetry code: (i) $x+\frac{1}{2}, -y, z$.

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalClear* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV5271).

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supplementary materials

Acta Cryst. (2012). E**68**, o1366 [doi:10.1107/S1600536812014067]

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Comment

The reported here crystal structure of the title compound, $C_{12}H_{11}NO_2$, represents a new orthorhombic polymorph (II)of the previously reported orthorhombic form (I) (Zhang *et al.* 2009). It was crystalized from a methanol solution of the title compound and (*R*)-2-(4-(carboxymethoxy)phenoxy)propanoic acid mixture.

In polymorph II (Figure 1), two six-membered rings form a dihedral angle of 13.8 (1)° [71.6 (1)° in I], and intermolecular O—H···N hydrogen bonds link molecules into chains along [100] (Figure 2, Table 1), in spite of hydrogen-bonded centrosymmetric dimers in polymorph I.

Experimental

The 2-(pyridin-4-ylmethoxy)phenol was synthesized by the reaction of *o*-benzenediol and 4-chloromethylpyridine hydrochloride under nitrogen atmosphere and alkaline condition (Gao *et al.*, 2004). Colourless block crystals were obtained by slow evaporation of a methanol solution (10 mL) containing title compound (0.402 g, 2 mmol) and (*R*)-2-(4-(carboxymethoxy)phenoxy)propanoic acid (0.48 g, 2 mmol) which only contained the molecules of title compound.

Refinement

H atoms bound to C atoms and the H atoms of the hydroxyl groups were placed in calculated positions and treated as riding on their parent atoms, with C—H = 0.93 Å (aromatic), C—H = 0.97 Å (methylene), O—H = 0.82 Å and with $U_{iso}(H) = 1.2U_{eq}(C)$, $U_{iso}(H) = 1.5U_{eq}(O)$.

Computing details

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO* (Rigaku, 1998); data reduction: *CrystalClear* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXL97* (Sheldrick, 2008).

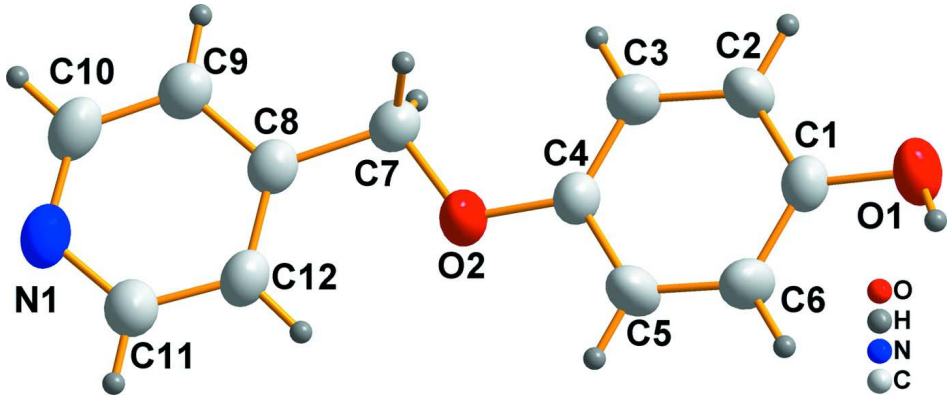

Figure 1

The molecular structure of the title compound, showing displacement ellipsoids at the 50% probability level for non-H atoms.

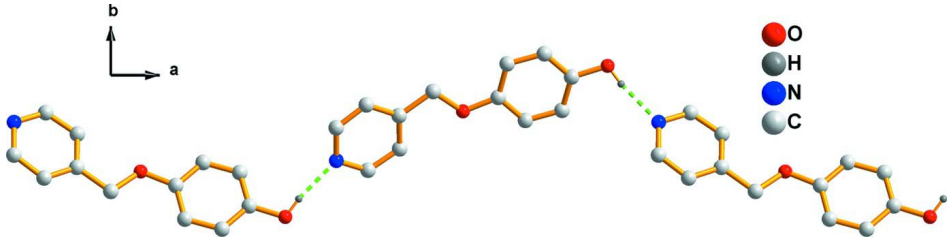

Figure 2

A partial packing view, showing hydrogen-bonded (dashed lines) chain structure along [100].

2-(pyridin-4-ylmethoxy)phenol

Crystal data

$C_{12}H_{11}NO_2$
$M_r = 201.22$
Orthorhombic, $Pca2_1$
Hall symbol: P 2c -2ac
$a = 23.398$ (5) Å
$b = 5.8343$ (12) Å
$c = 7.3934$ (15) Å
$V = 1009.3$ (4) Å^3
$Z = 4$
$F(000) = 424$
$D_x = 1.324$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 5894 reflections
$\theta = 3.3$–27.5°
$\mu = 0.09$ mm^{-1}
$T = 293$ K
Block, colourless
0.50 × 0.37 × 0.11 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scan
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min} = 0.956$, $T_{max} = 0.990$
8907 measured reflections
2285 independent reflections
1298 reflections with $I > 2\sigma(I)$
$R_{int} = 0.066$
$\theta_{max} = 27.5°$, $\theta_{min} = 3.3°$
$h = -30 \rightarrow 30$
$k = -7 \rightarrow 7$
$l = -9 \rightarrow 9$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.043$
$wR(F^2) = 0.077$
$S = 1.01$
2285 reflections
138 parameters
1 restraint
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0218P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.15$ e Å^{-3}
$\Delta\rho_{min} = -0.14$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0028 (6)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.68990 (6)	0.4700 (3)	0.0425 (3)	0.0567 (5)
H1	0.7109	0.3578	0.0381	0.085*
O2	0.46554 (6)	0.1873 (3)	−0.0201 (2)	0.0566 (5)
N1	0.26917 (7)	−0.1195 (3)	0.0264 (3)	0.0488 (5)
C2	0.59170 (9)	0.5453 (4)	0.0842 (3)	0.0442 (6)
H2	0.6014	0.6865	0.1339	0.053*
C8	0.36646 (8)	0.1609 (4)	0.0395 (3)	0.0390 (5)
C7	0.41925 (8)	0.3104 (4)	0.0562 (3)	0.0429 (6)
H7A	0.4137	0.4538	−0.0078	0.052*
H7B	0.4269	0.3444	0.1824	0.052*
C12	0.36737 (9)	−0.0462 (4)	−0.0507 (3)	0.0448 (6)
H12	0.4003	−0.0958	−0.1091	0.054*
C3	0.53418 (9)	0.4830 (4)	0.0713 (3)	0.0461 (6)
H3	0.5057	0.5825	0.1107	0.055*
C4	0.52013 (8)	0.2740 (4)	0.0000 (3)	0.0410 (6)
C1	0.63411 (8)	0.4011 (4)	0.0247 (3)	0.0403 (5)
C6	0.61922 (9)	0.1936 (4)	−0.0516 (4)	0.0518 (6)
H6	0.6475	0.0958	−0.0948	0.062*
C9	0.31568 (9)	0.2274 (4)	0.1199 (3)	0.0463 (6)
H9	0.3132	0.3668	0.1804	0.056*
C10	0.26894 (9)	0.0849 (4)	0.1093 (3)	0.0499 (7)
H10	0.2351	0.1333	0.1629	0.060*
C5	0.56238 (9)	0.1309 (4)	−0.0638 (4)	0.0541 (7)
H5	0.5526	−0.0089	−0.1156	0.065*

C11	0.31825 (8)	−0.1789 (4)	−0.0526 (3)	0.0485 (6)
H11	0.3196	−0.3186	−0.1131	0.058*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0343 (8)	0.0535 (11)	0.0821 (13)	−0.0041 (7)	−0.0031 (10)	0.0010 (11)
O2	0.0315 (8)	0.0521 (10)	0.0861 (14)	−0.0023 (7)	0.0054 (9)	−0.0184 (11)
N1	0.0361 (10)	0.0534 (13)	0.0569 (12)	0.0003 (10)	0.0028 (10)	0.0084 (12)
C2	0.0414 (13)	0.0342 (13)	0.0569 (17)	−0.0032 (10)	−0.0020 (12)	−0.0076 (12)
C8	0.0350 (11)	0.0406 (13)	0.0416 (13)	0.0046 (10)	−0.0013 (11)	0.0052 (12)
C7	0.0378 (12)	0.0438 (13)	0.0472 (15)	0.0026 (10)	0.0045 (12)	−0.0016 (14)
C12	0.0333 (12)	0.0500 (15)	0.0510 (14)	0.0030 (11)	0.0049 (12)	0.0009 (14)
C3	0.0413 (13)	0.0392 (14)	0.0577 (16)	0.0057 (11)	0.0009 (13)	−0.0070 (13)
C4	0.0313 (11)	0.0430 (13)	0.0487 (14)	0.0001 (10)	0.0011 (10)	−0.0034 (12)
C1	0.0329 (11)	0.0421 (13)	0.0460 (14)	−0.0004 (10)	0.0000 (12)	0.0045 (13)
C6	0.0375 (12)	0.0489 (15)	0.0690 (17)	0.0089 (11)	0.0008 (14)	−0.0165 (15)
C9	0.0425 (13)	0.0437 (15)	0.0528 (15)	0.0036 (12)	0.0052 (11)	0.0025 (13)
C10	0.0367 (13)	0.0554 (17)	0.0577 (16)	0.0096 (12)	0.0054 (12)	0.0097 (15)
C5	0.0424 (13)	0.0429 (14)	0.0771 (18)	−0.0008 (11)	−0.0026 (14)	−0.0206 (16)
C11	0.0432 (12)	0.0516 (16)	0.0506 (14)	−0.0007 (12)	0.0004 (12)	−0.0006 (14)

Geometric parameters (Å, º)

O1—C1	1.372 (2)	C12—C11	1.386 (3)
O1—H1	0.8200	C12—H12	0.9300
O2—C4	1.382 (2)	C3—C4	1.368 (3)
O2—C7	1.417 (2)	C3—H3	0.9300
N1—C11	1.334 (3)	C4—C5	1.377 (3)
N1—C10	1.340 (3)	C1—C6	1.380 (3)
C2—C1	1.373 (3)	C6—C5	1.382 (3)
C2—C3	1.397 (3)	C6—H6	0.9300
C2—H2	0.9300	C9—C10	1.376 (3)
C8—C12	1.381 (3)	C9—H9	0.9300
C8—C9	1.384 (3)	C10—H10	0.9300
C8—C7	1.517 (3)	C5—H5	0.9300
C7—H7A	0.9700	C11—H11	0.9300
C7—H7B	0.9700		

C1—O1—H1	109.5	C3—C4—C5	119.98 (18)
C4—O2—C7	118.54 (17)	C3—C4—O2	126.16 (19)
C11—N1—C10	115.8 (2)	C5—C4—O2	113.8 (2)
C1—C2—C3	121.0 (2)	O1—C1—C2	118.5 (2)
C1—C2—H2	119.5	O1—C1—C6	122.45 (19)
C3—C2—H2	119.5	C2—C1—C6	119.08 (19)
C12—C8—C9	117.8 (2)	C1—C6—C5	120.1 (2)
C12—C8—C7	122.01 (19)	C1—C6—H6	119.9
C9—C8—C7	120.2 (2)	C5—C6—H6	119.9
O2—C7—C8	107.36 (18)	C10—C9—C8	119.2 (2)
O2—C7—H7A	110.2	C10—C9—H9	120.4

C8—C7—H7A	110.2	C8—C9—H9	120.4
O2—C7—H7B	110.2	N1—C10—C9	124.1 (2)
C8—C7—H7B	110.2	N1—C10—H10	118.0
H7A—C7—H7B	108.5	C9—C10—H10	118.0
C8—C12—C11	118.8 (2)	C4—C5—C6	120.5 (2)
C8—C12—H12	120.6	C4—C5—H5	119.7
C11—C12—H12	120.6	C6—C5—H5	119.7
C4—C3—C2	119.3 (2)	N1—C11—C12	124.4 (2)
C4—C3—H3	120.3	N1—C11—H11	117.8
C2—C3—H3	120.3	C12—C11—H11	117.8

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N1^{i}	0.82	1.95	2.763 (2)	173

Symmetry code: (i) *x*+1/2, −*y*, *z*.